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(CLEAN FORM)

1. A method for use in deriving fixed bond information, comprising:

analyzing a Kekulé structure representation of a chemical structure;

identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluating at least a subset of the fixed bond representation candidates;

selecting from among the plurality of fixed bond representation candidates based on the evaluation; and

producing fixed bond information based on the selection.

2. A system for use in deriving fixed bond information, comprising:

an analyzer analyzing a Kekulé structure representation of a chemical structure;

an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

an evaluator evaluating at least a subset of the fixed bond representation candidates;

a selector electing from among the plurality of fixed bond representation candidates based on the evaluation; and

a producer producing fixed bond information based on the selection.

3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:

analyze a Kekulé structure representation of a chemical structure;

identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;

evaluate at least a subset of the fixed bond representation candidates; and

select from among the plurality of fixed bond representation candidates based on the evaluation; and

produce fixed bond information based on the selection.

4. The method of claim 1, wherein at least a portion of the Kekulé structure representation describes a monocyclic ring system.

5. The method of claim 1, wherein at least a portion of the Kekulé structure representation describes a polycyclic ring system.

6. The method of claim 1, wherein at least a portion of the Kekulé structure representation describes a ring system with a hetero substitution pattern.

7. The method of claim 1, wherein at least a portion of the Kekulé structure representation describes a non-cyclic system.

8. The method of claim 1, wherein at least a portion of the Kekulé structure representation describes an acyclic system.

9. The method of claim 1, further comprising:

based on the fixed bond information, producing a fixed bond representation that includes a pair of opposite charges lacked by the Kekulé structure representation.

10. The method of claim 1, further comprising:

based on the fixed bond information, producing a fixed bond representation that includes a pair of radicals lacked by the Kekulé structure representation.

11. The method of claim 1, further comprising:

queuing at least a subset of the candidates by priority.

12. The method of claim 1, further comprising:

using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the Kekulé structure representation.

13. The method of claim 12, wherein the table is configured to allow additional elements and values to be added.

14. The method of claim 12, wherein the table is configured to allow additional elements and values to be added to apply to any chemical element.

15. The method of claim 1, further comprising:

deriving electronic state and valence distributions information together with analyzing the Kekulé structure representation.

16. The method of claim 1, further comprising:

determining whether it is practical to produce a fixed bond representation of the chemical structure.

17. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18. The method of claim 1, further comprising:

determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.